Supplementary information

for

Photoelectrochemical water splitting by Hematite boosted in heterojunction with B-doped g-C_3N_4 nanosheets and carbon nanotubes

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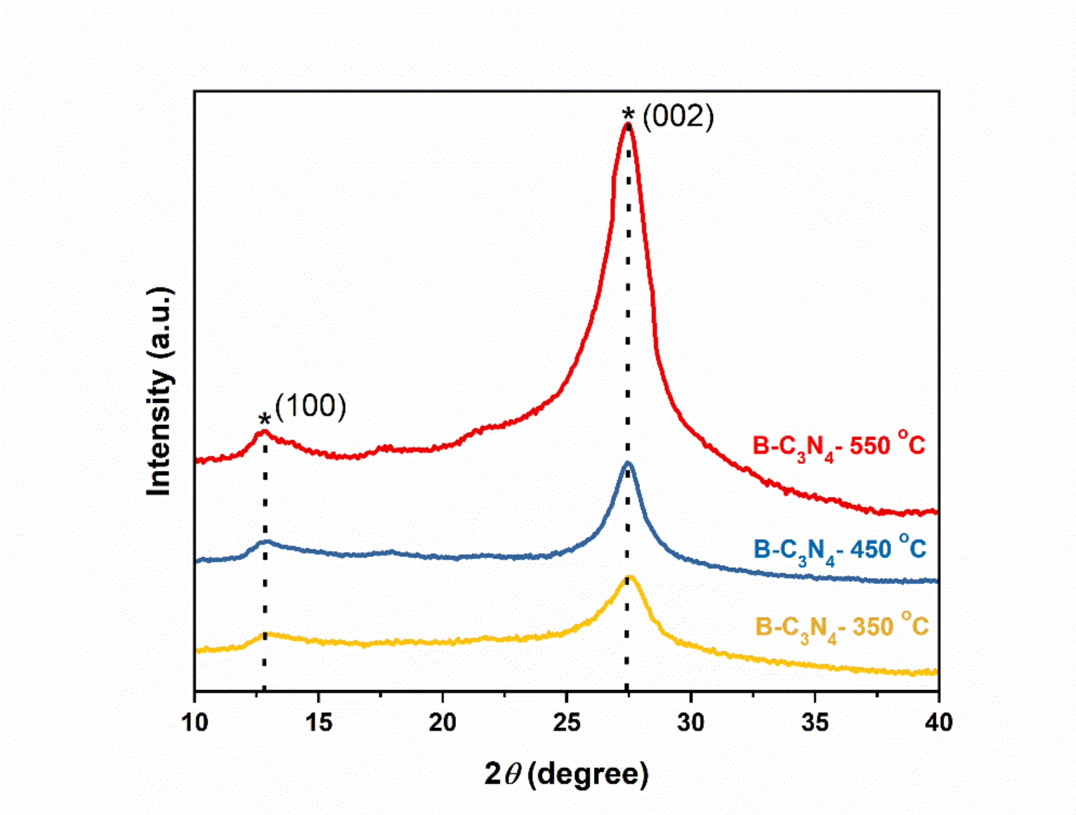

Figure S1. XRD of the B-C_3N_4 samples used in our study with the two expected reflections as discussed in the main text.

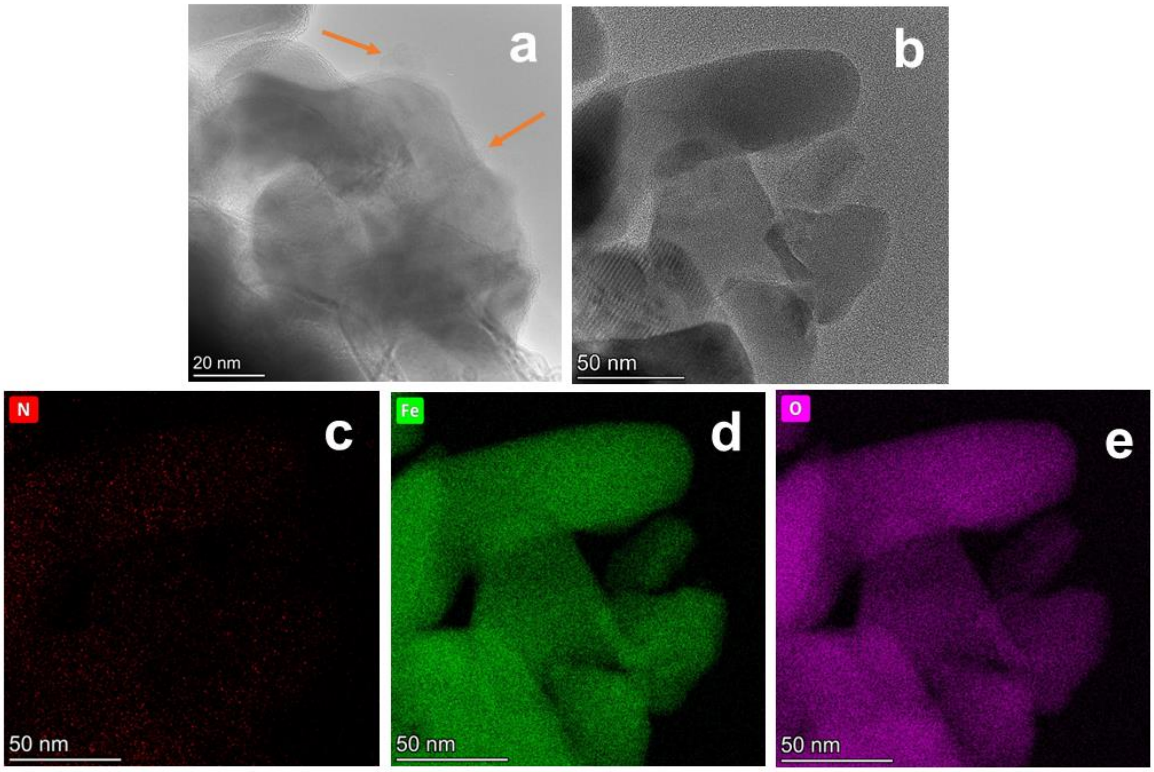

Figure S2. HRTEM and STEM-EDS images of the used α-Fe_2O_3/B-C_3N_4/p-CNT composite (a-b) showed partial crystalline and amorphous structures layered on the α-Fe_2O_3 surface; (c-e) unveiled the homogeneous distribution of nitrogen (N), iron (Fe) and oxygen (O) species across the entirety of the nanorod structures, affirming the successful integration of B-C_3N_4 dopants into the hematite matrix.

Table S1. Surface atomic concentrations (%) of the used photoanodes were calculated from XPS data.

	Surface atomic concentrations (%)		
	***a*-Fe_2O_3**	***a*-Fe_2O_3 / B-C_3N_4**	***a*-Fe_2O_3 / B-C_3N_4 / p-CNT**
B 1s	1.09	1.03	0.94
C 1s	9.71	10.4	5.7
Cl 2p	0.16	0.2	0.12
Fe 2p	31.94	31.36	35.02
N 1s	0.36	1.09	0.73
Na 1s	2.37	1.89	1.74
O 1s	52.43	52.17	54.42
S 2p	0.91	1.26	1.1
Ti 2p	1.03	0.61	0.23

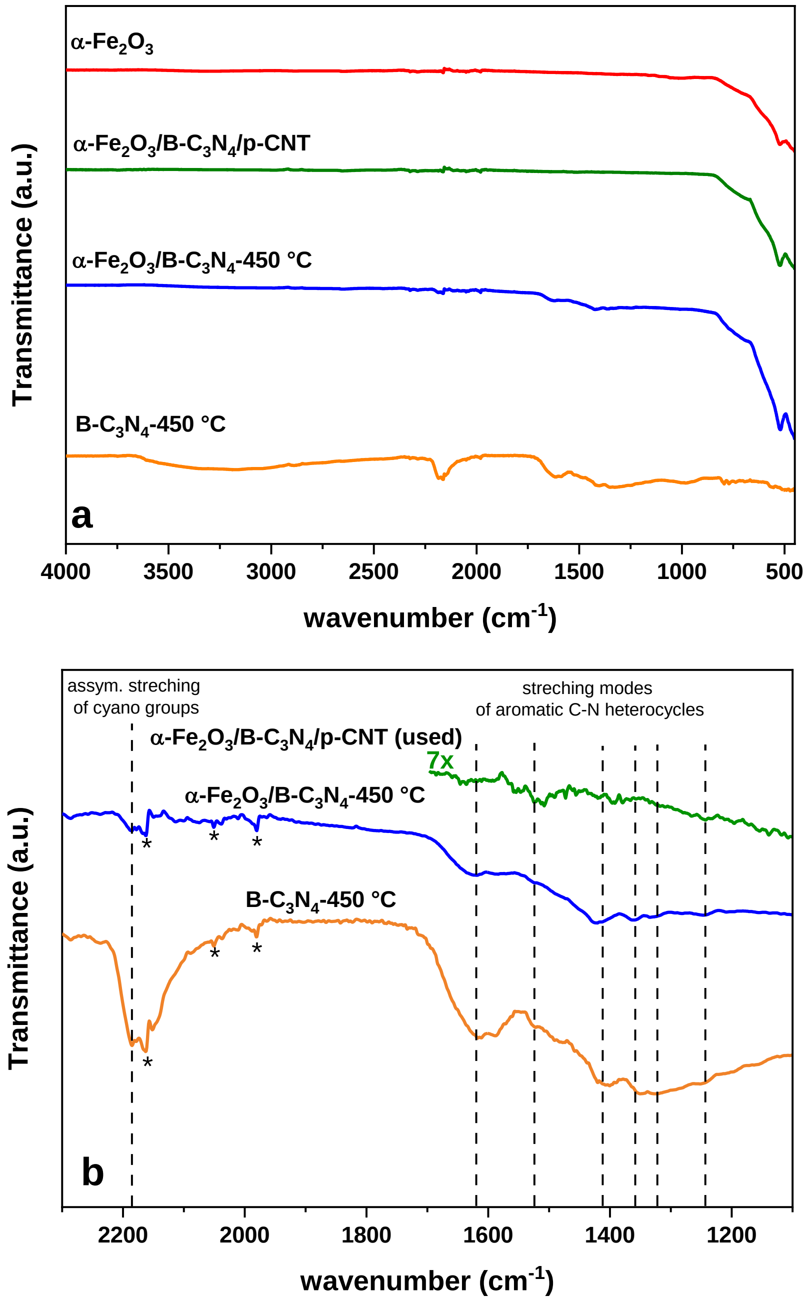

Figure S3. (a) ATR-IR spectra of as-synthesized B-C_3N_4-450 °C, α-Fe_2O_3 and α-Fe_2O_3/B-C_3N_4-450 °C (enriched twice in B-C_3N_4-450 °C for the analysis), and the used α-Fe_2O_3/B-C_3N_4-450 °C/p-CNT photoanodes; (b) corresponding magnified range of 1100–2300 cm^{-1}. Characteristic stretching modes correspond with a more detailed analysis of B-C_3N_4, in the ESI of ref. [47]. Asterisks assign artefacts of the diamond detector of the ATR.

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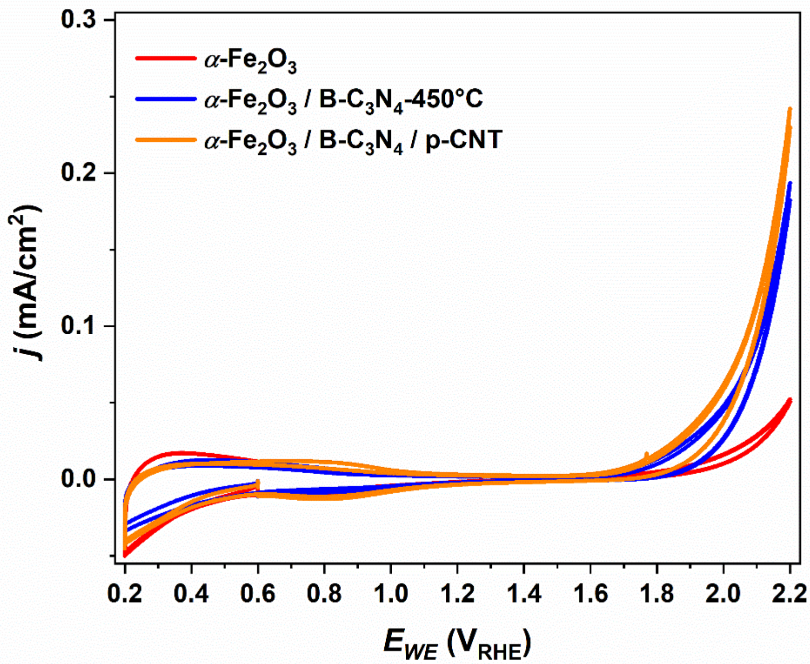

Figure S4. Cyclic voltammetry of the photoanodes used in photoelectrochemistry as shown in Figure 4, recorded in the dark, 2 cycles at 5 mVs^{-1} in 0.1 M Na_2SO_4 at pH 7.

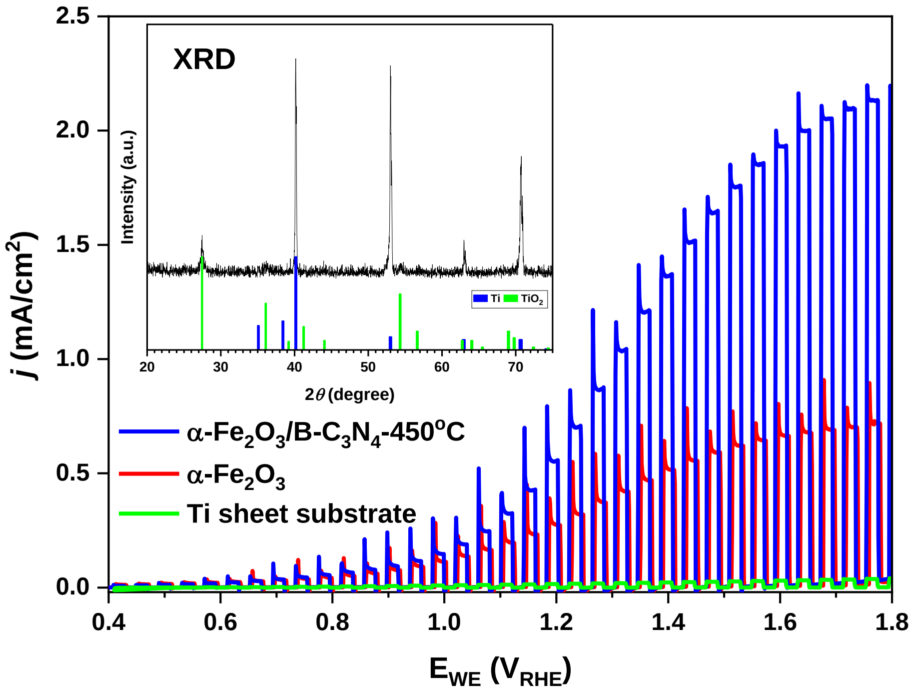

Figure S5. Comparative Linear sweep voltammetry plots between uncoated Ti sheet, pristine α-Fe_2O_3, α-Fe_2O_3/B-C_3N_4-450 °C obtained in 0.1 M Na_2SO_4 at pH 7. The inset shows the XRD patterns of the uncoated Ti substrate.

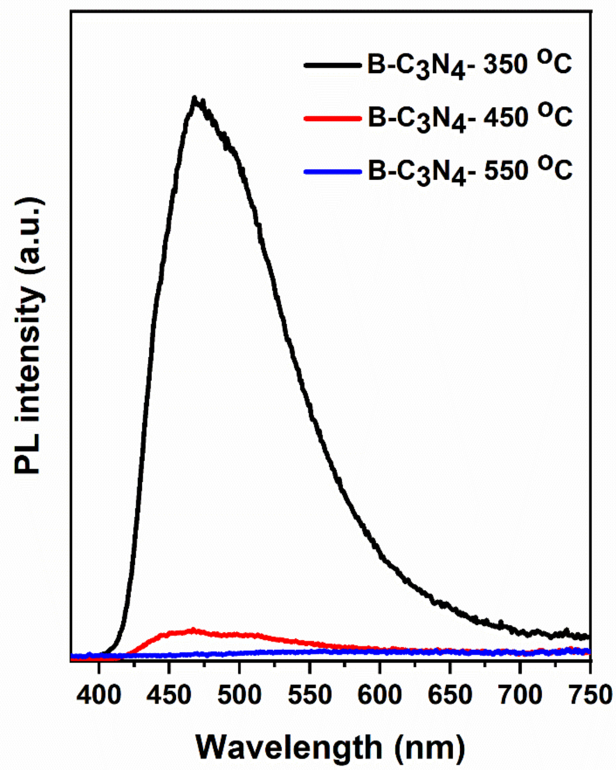

Figure S6. PL spectra of B-C_3N_4 samples at different heat-treatment temperatures.

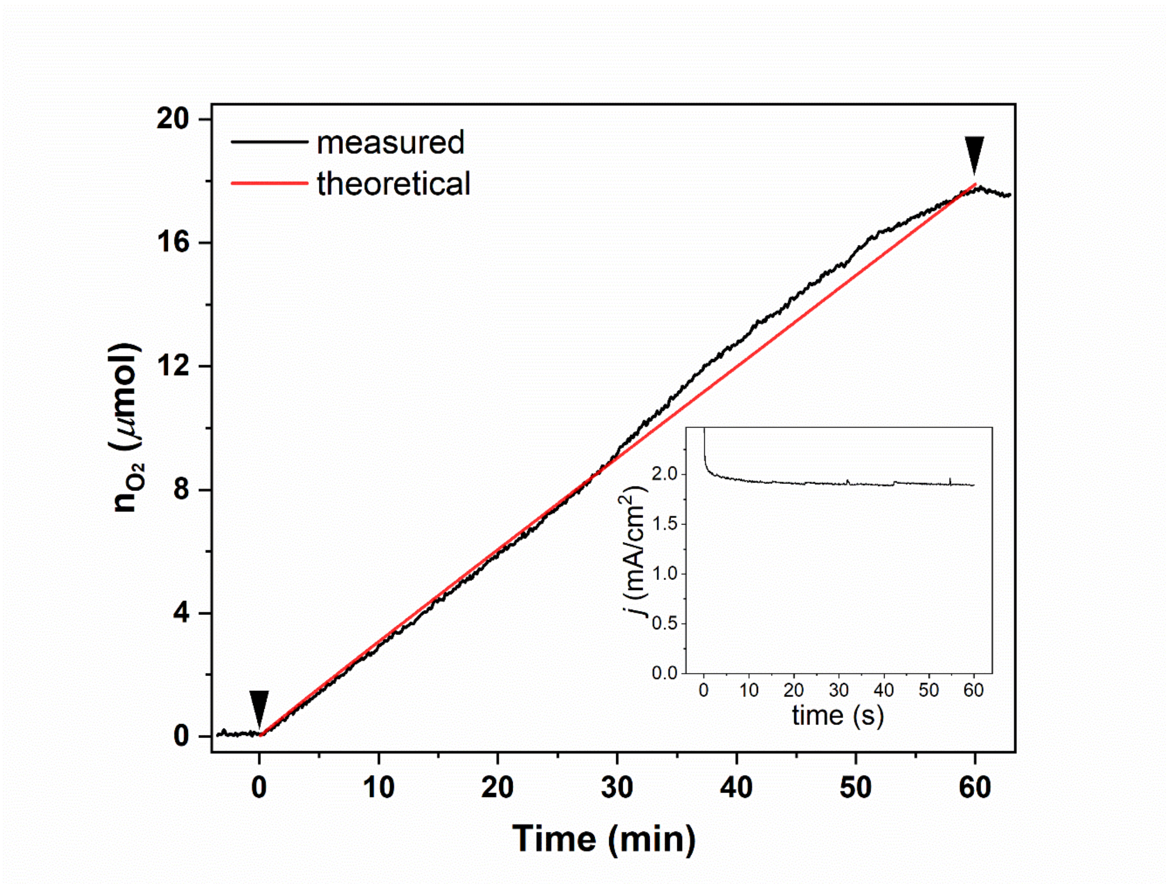

Figure S7. Detected oxygen (black line) and the theoretical amount (red line) in the course of a 1-hour CPE experiment at 1.7 V_{RHE} reference electrode and irradiation at 100 mW cm^{-2} in 0.1 M Na_2SO_4 at pH 7 using the α-Fe_2O_3/B-C_3N_4 -450 °C/p-CNT photoanode. The theoretical amount of produced oxygen was calculated from the charge as $n_{O2} = Q/4F$, where n is the molar amount of O_2, Q is the passed charge in Coulombs, F is the Faraday constant, 96485 C/mol. The black marks indicate the start and the end of the CPE experiment. **Inset:** current density during the experiment.

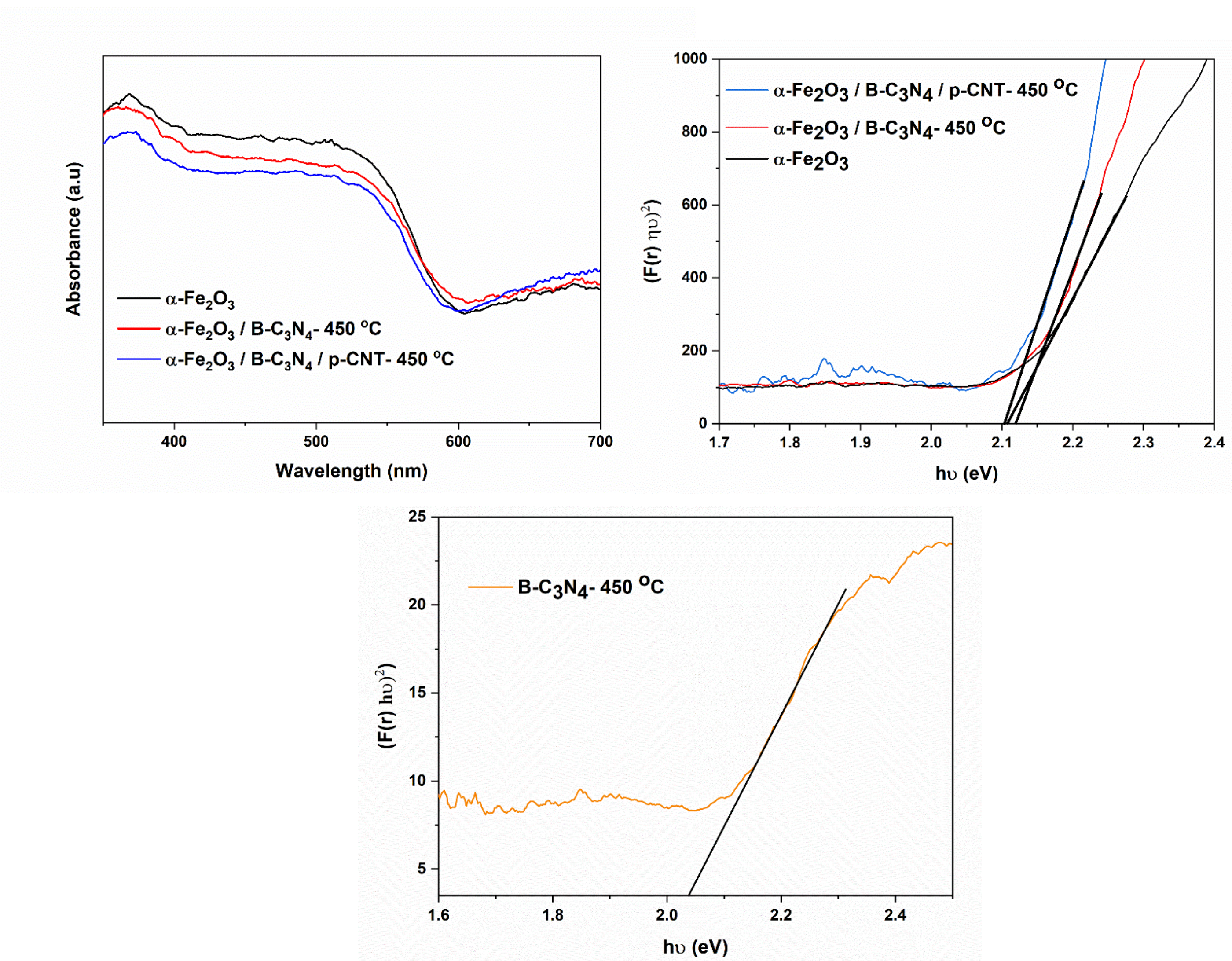

Figure S8. Optical absorbance spectra (DRS) and Tauc plots for the samples as indicated in the legend. The optical absorption ability of α-Fe_2O_3/B-C_3N_4-450 °C/p-CNT was unchanged, and the remarkable PEC enhancement should be attributed to the surface charge property modification by B-C_3N_4-450 °C and p-CNT decoration. The UV-vis spectra have very little difference among all the photoanodes, indicating the negligible influence of B-C_3N_4-450 °C and/or p-CNT decoration on the optical absorption of hematite due to the low loadings. The absorption edges of α-Fe_2O_3, α-Fe_2O_3/B-C_3N_4-450 °C, and α-Fe_2O_3/B-C_3N_4-450 °C/p-CNT are located *ca*. 590 nm, and the corresponding bandgaps (E_g) of the corresponding samples are calculated by Tauc method to be ca. 2.10 eV and 2.04 eV for B-C_3N_4 -450 °C.

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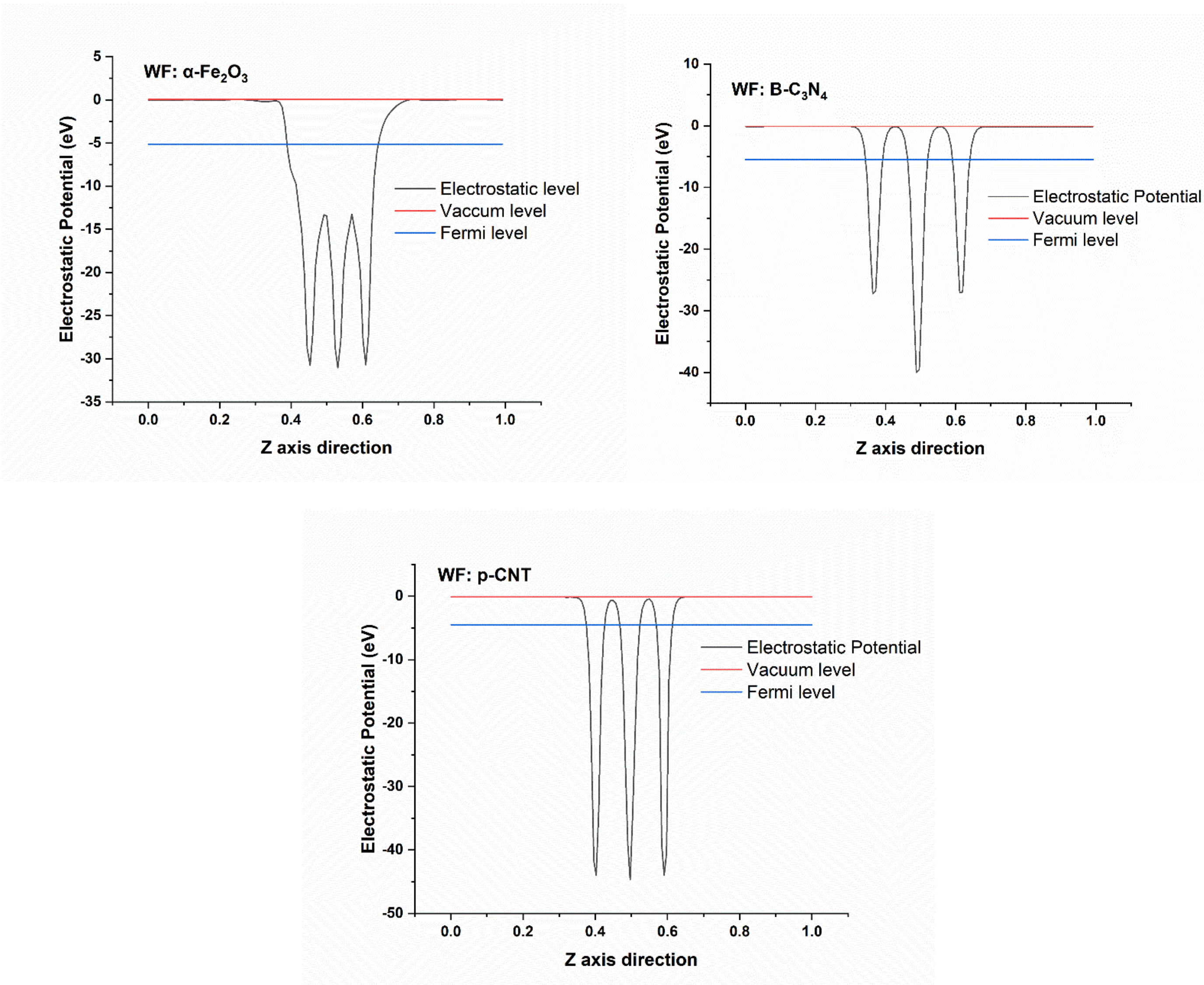

Figure S9. The work functions as calculated for α-Fe_2O_3, B-C_3N_4, and p-CNT are 5.18, 5.39, and 4.18 eV.